Black Box Variational Inference with a Deterministic Objective

Faster, More Accurate, and Even More Black Box

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Problem statement

We all want to do accurate Bayesian inference quickly:

- In terms of compute (wall time, model evaluations, parallelism)
- In terms of analyst effort (tuning, algorithmic complexity)

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Black Box Variational Inference (BBVI) can be faster alternative to MCMC. **But...**

- BBVI is cast as an optimization problem with an intractable objective $\Rightarrow$
- Most BBVI methods use **stochastic gradient** (SG) optimization $\Rightarrow$
  - SG algorithms can be hard to tune
  - Assessing convergence and stochastic error can be difficult
  - SG optimization can perform worse than second-order methods on tractable objectives
- Many BBVI methods employ a **mean-field (MF) approximation** $\Rightarrow$
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Our proposal: replace the intractable BBVI objective with a fixed approximation.

- Better optimization methods can be used (e.g. true second-order methods)
- Convergence and approximation error can be assessed directly
- Can correct posterior covariances with linear response covariances
- This technique is well-studied (but there's still work to do in the context of BBVI)

$\Rightarrow$ **Simpler, faster, and better BBVI posterior approximations ... in some cases.**

Outline

- BBVI Background and our proposal
  - Automatic differentiation variational inference (ADVI) (a BBVI method)
  - Our approximation: "Deterministic ADVI" (DADVI)
  - Linear response (LR) covariances
  - Estimating approximation error
- Experimental results: DADVI vs ADVI
  - DADVI converges faster than ADVI, and requires no tuning
  - DADVI's posterior mean estimates' accuracy are comparable to ADVI
  - DADVI+LR provides more accurate posterior variance estimates than ADVI
  - DADVI provides accurate estimates of its own approximation error
  - But stochastic ADVI often results in better objective function values (eventually)
- Theory and shortcomings
  - Pessimistic dimension dependence results from optimization theory
  - ...which do not apply in certain BBVI settings.
  - DADVI fails for expressive BBVI approximations (e.g. full-rank ADVI)
  - More work to be done!

Notation

$$\begin{aligned} \text{Data:} \quad & y \\ \text{Likelihood:} \quad & \mathcal{P}(y|\theta) \\ \text{Parameter:} \quad & \theta \in \mathbb{R}^{D_\theta} \\ \text{Prior:} \quad & \mathcal{P}(\theta) \quad \text{(density w.r.t. Lebesgue } \mathbb{R}^{D_\theta}\text{, nonzero everywhere)} \end{aligned}$$

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Example: Election modeling (2016 US POTUS)

Data y :	Polling data (colored dots)
Likelihood $\mathcal{P}(y\|\theta)$:	Time series with random effects
Parameter θ :	15, 098-dimensional
Interested in:	Vote share on election day
MCMC time:	643 minutes (PyMC3 NUTS)

How can we approximate the posterior more quickly?
One answer: variational inference.

Variational inference [Blei et al., 2016]

We want the posterior $\mathcal{P}(\theta|y)$. Let $\mathrm{KL}\left(\mathcal{Q}(\theta)||\mathcal{P}(\theta)\right)$ denote KL divergence:

$$\mathrm{KL}\left(\mathcal{Q}(\theta)||\mathcal{P}(\theta)\right) = \mathop{\mathbb{E}}_{\mathcal{Q}(\theta)}\left[\log \mathcal{Q}(\theta)\right] - \mathop{\mathbb{E}}_{\mathcal{Q}(\theta)}\left[\log \mathcal{P}(\theta)\right].$$

The KL divergence is zero if and only if the two distributions are the same.

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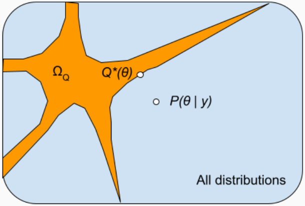

We hope to choose $\Omega_{\mathcal{Q}}$ so that

- The optimization problem is tractable
  - $\rightarrow$ simple $\Omega_{\mathcal{Q}}$ are better
- The best approximation is a good one
  - $\rightarrow$ complex $\Omega_{\mathcal{Q}}$ are better

The approximation can be poor because

- Poor optimization
- The family $\Omega_{\mathcal{Q}}$ isn't expressive enough

When does variational inference work?

When, in general, is $\overset{*}{\mathcal{Q}}(\theta)$ a good approximation for a given family $\Omega_{\mathcal{Q}}$?

It is hard to say.

Black-box variational inference

To perform VI, we need to solve

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How can we optimize this objective? **Black-box VI [Ranganath et al., 2014]:**

- Parameterize the family $\Omega_{\mathcal{Q}}$ using $\eta \in \mathbb{R}^{D_\eta}$ (so we have $\mathcal{Q}(\theta|\eta)$)
  - We will study **ADVI**, which takes $\mathcal{Q}(\theta|\eta)$ to be Gaussian [Kucukelbir et al., 2017].
  - The parameters η are the means and covariance ("mean-field" or "full-rank")
- Re-write the objective (using the reparameterization trick) as

$$\underset{\eta}{\mathrm{argmin}}\, F(\eta) \quad \text{where} \quad F(\eta) := \underset{\mathcal{N}_{\mathrm{std}}(z)}{\mathbb{E}}\left[f(\eta, z)\right].$$

- Use autodiff to differentiate $\eta \mapsto f(\eta, z)$
- Optimize with stochastic optimization using draws $z_n \sim \mathcal{N}_{\mathrm{std}}(z)$.

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We propose:

Instead of $\underset{\mathcal{N}_{\mathrm{std}}(z)}{\mathbb{E}} [f(\eta, z)]$, optimize $\frac{1}{N} \sum_{n=1}^{N} f(\eta, z_n)$ for fixed $z_n \overset{iid}{\sim} \mathcal{N}_{\mathrm{std}}(z)$.

Two approaches

$$\text{Consider} \quad \operatorname*{argmin}_{\eta} F(\eta) \quad \text{where} \quad F(\eta) := \mathop{\mathbb{E}}_{\mathcal{N}_{\mathrm{std}}(z)} \left[f(\eta, z) \right].$$

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Algorithm 1

Stochastic gradient (SG)

ADVI (and most BBVI)

Fix N (typically $N = 1$)
$t \leftarrow 0$
while Not converged **do**
  $t \leftarrow t + 1$
  Draw $\mathcal{Z}_N$
  $\Delta_S \leftarrow \nabla_\eta \hat{F}(\eta_{t-1}|\mathcal{Z}_N)$
  $\alpha_t \leftarrow \mathrm{SetStepSize}(\text{Past state})$
  $\eta_t \leftarrow \eta_{t-1} - \alpha_t \Delta_S$
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end while
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Algorithm 2
Sample average approximation (SAA)
Deterministic ADVI (DADVI) (proposal)

- Fix N (our experiments use $N = 30$)
- Draw $\mathcal{Z}_N$
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Our proposal: Apply Algorithm 2 with the ADVI objective.
Take better steps, easily assess convergence, with less tuning.

Experiments

For each of a range of models (next slide), we compared:

- **NUTS:** The "no-U-turn" MCMC sampler as implemented by PyMC [Salvatier et al., 2016]. We used this as the "ground truth" posterior.

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Stochastic ADVI methods:

- Mean field ADVI: We used the PyMC implementation of ADVI, together with its default termination criterion (based on parameter differences).
- Full-rank ADVI: We used the PyMC implementation of full-rank ADVI, together with the default termination criterion for ADVI described above.
- RAABBVI: To run RAABBVI, we used the public package `viabel`, provided by Welandawe et al. [2022].

We terminated unconverged stochastic ADVI after 100,000 iterations.

We evaluated each method on a range of models.

Model Name	Dim D_θ	NUTS runtime	Description
ARM (53 models)	Median 5 (max 176)	median 39 seconds (max 16 minutes)	A range of linear models, GLMs, and GLMMs
Microcredit	124	597 minutes	Hierarchical model with heavy tails and zero inflation
Occupancy	$1,884$	251 minutes	Binary regression with highly crossed random effects
Tennis	$5,014$	57 minutes	Binary regression with highly crossed random effects
POTUS	$15,098$	643 minutes	Autoregressive time series with random effects

Table 1: Model summaries.

Comparisons

To form a common scale for the accuracy of the posteriors, we report:

$$\varepsilon^{\mu}_{\text{METHOD}} := \frac{\mu_{\text{METHOD}} - \mu_{\text{NUTS}}}{\sigma_{\text{NUTS}}} \qquad \varepsilon^{\sigma}_{\text{METHOD}} := \frac{\sigma_{\text{METHOD}} - \sigma_{\text{NUTS}}}{\sigma_{\text{NUTS}}}.$$

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We measure computational cost using both

- **Wall time** and
- **Number of model evaluations** (gradients, Hessian-vector products).

We compare achieved objective values using a large number of independent samples.

We report objective values and computation cost relative to DADVI.

Posterior mean accuracy

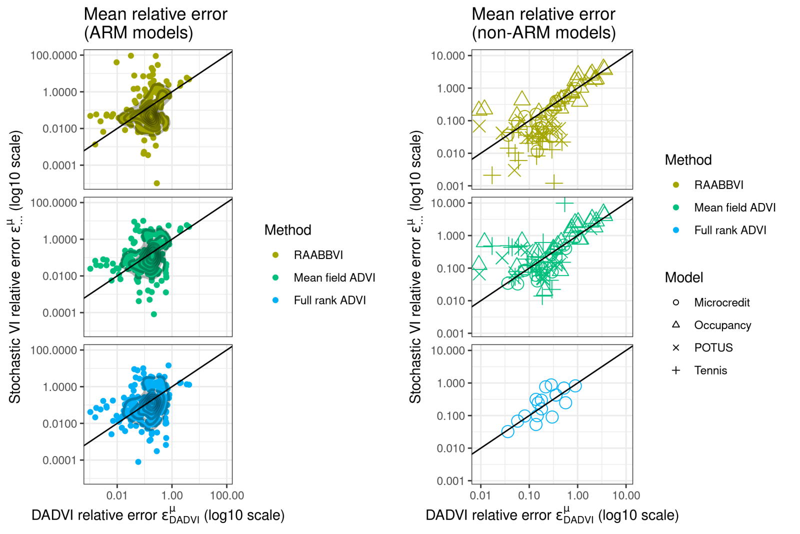

Figure 1: Posterior mean accuracy (relative to MCMC posterior standard deviation). Each point is a single named parameter in a single model. Points above the diagonal line indicate better DADVI or LRVB performance.

Computational cost for ARM models

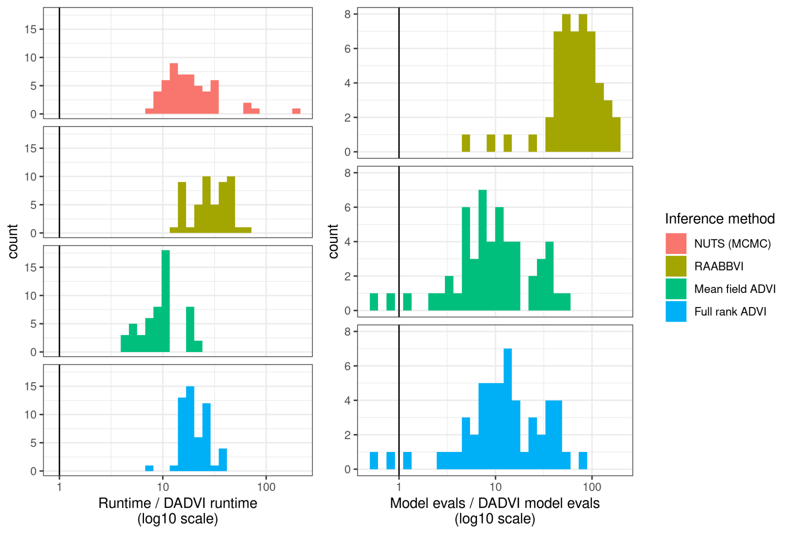

Figure 2: Runtimes and model evaluation counts for the ARM models. Results are reported divided by the corresponding value for DADVI.

Computational cost for non-ARM models

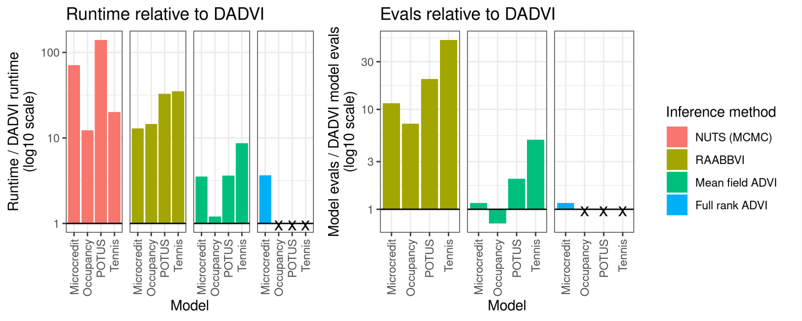

Figure 3: Runtimes and model evaluation counts for the non-ARM models. Results are reported divided by the corresponding value for DADVI. Missing model / method combinations are marked with an X.

Optimization traces for ARM models

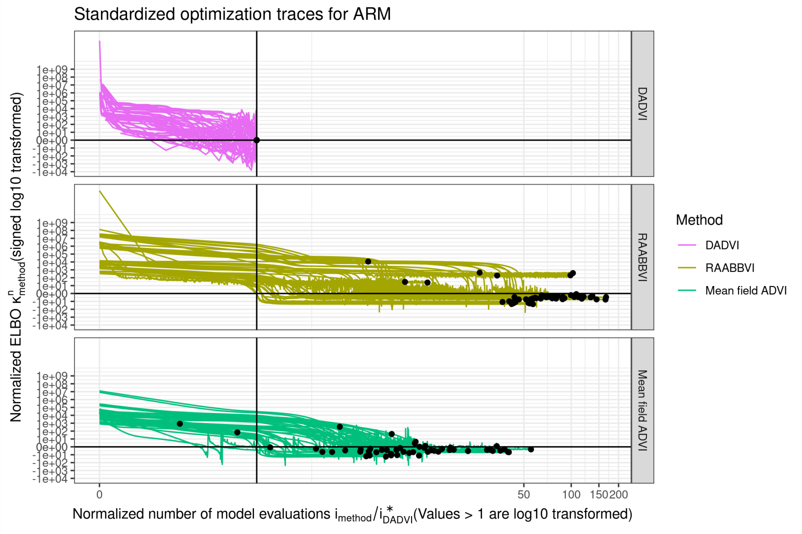

Figure 4: Optimization traces for the ARM models. Black dots show the termination point of each method. Dots above the horizontal black line mean that DADVI found a better ELBO. Dots to the right of the black line mean that DADVI terminated sooner in terms of model evaluations.

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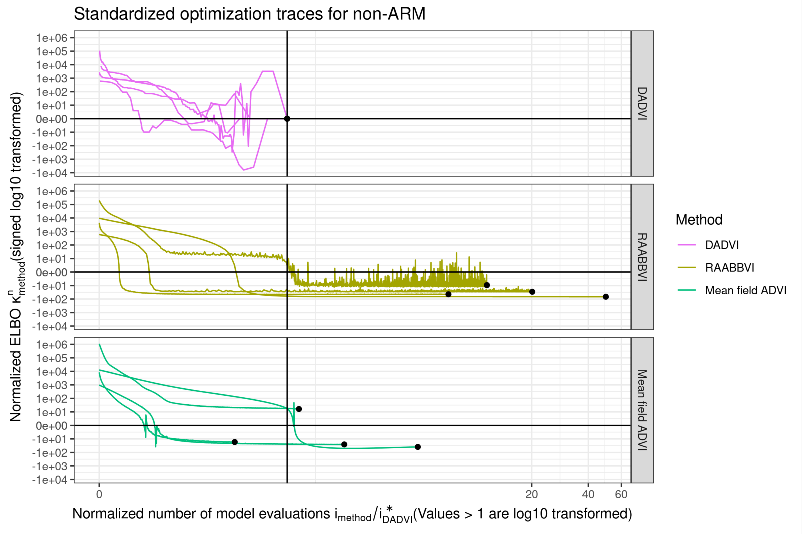

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Experiment summary

$\Rightarrow$ DADVI is faster, simpler, and the posterior means are not worse.

But DADVI can additionally provide:

- Simple estimates of approximation error
- Improved (LR) posterior covariance esimates

Linear response covariances and sampling uncertainty

Intractable objective:

$$\overset{*}{\eta} = \underset{\eta \in \mathbb{R}^{D_\eta}}{\mathrm{argmin}} \underset{\mathcal{N}_{\mathrm{std}}(z)}{\mathbb{E}} \left[f(\eta, z) \right]$$

DADVI approximation:

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Answer: The same as a that of any M-estimator: asymptotically normal (as N grows)

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Linear response (LR) covariances improve covariance estimates by computing *sensitivity* of the variational means to particular perturbations. [Giordano et al., 2018]

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Both DADVI error and LR covariances can be computed from the DADVI objective.

Stochastic ADVI does not produce an actual optimum of any tractable objective, so LR and M-estimator computations are unavailable.

Posterior standard deviation accuracy

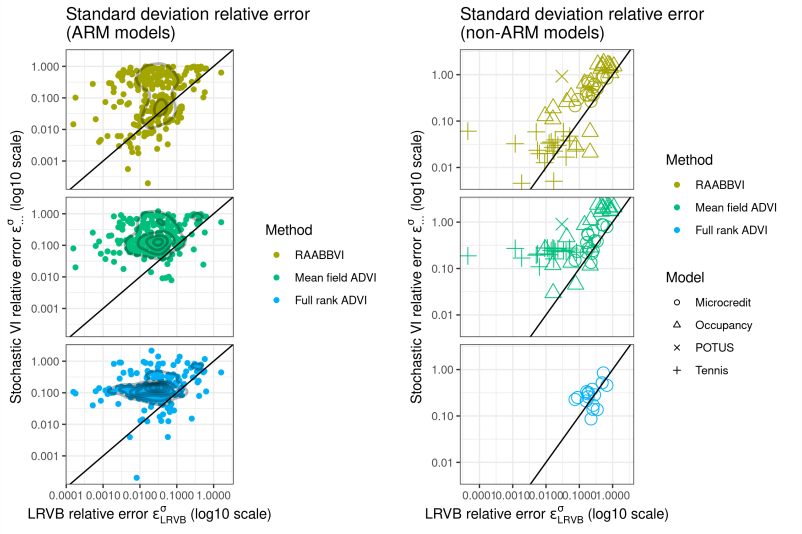

Figure 6: Posterior sd relative accuracy. Each point is a single named parameter in a single model. Points above the diagonal line indicate better DADVI or LRVB performance.

DADVI approximation error accuracy

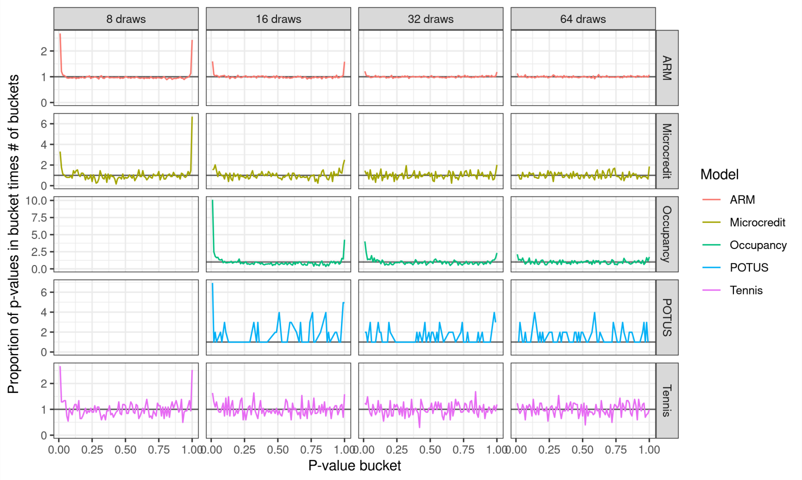

Figure 7: Density estimates of $\Phi(\varepsilon^{\xi})$ for difference models. All the ARM models are grouped together for ease of visualization. Each panel shows a binned estimate of the density of $\Phi(\varepsilon^{\xi})$ for a particular model and number of draws N. Values close to one (a uniform density) indicate good frequentist performance. CG failed for the Occupancy and POTUS models with only 8 draws, possibly indicating poor optimization performance with so few samples.

Previous theoretical results

Intractable objective:

$$\overset{*}{\eta} = \underset{\eta \in \mathbb{R}^{D_\eta}}{\mathrm{argmin}} \underset{\mathcal{N}_{\mathrm{std}}(z)}{\mathbb{E}} [f(\eta, z)]$$

SAA approximation (DADVI):

$$\hat{\eta}(\mathcal{Z}_N) = \underset{\eta \in \mathbb{R}^{D_\eta}}{\mathrm{argmin}} \frac{1}{N} \sum_{n=1}^{N} f(\eta, z_n).$$

The idea of optimizing $\hat{F}$ instead of SG on F is old and well-studied in the optimization literature, where $\hat{F}$ is known as the **Sample average approximation (SAA)**.

Yet SAA is rarely used for BBVI.[1] One possible reason is the following:

Theorem [Nemirovski et al., 2009]: In general, the error of both SG and SAA scale as $\sqrt{D_\theta / N}$, where, for SG, N is the *total number of samples used*.

[1] Some exceptions I'm aware of: Giordano et al. [2018, 2022], Wycoff et al. [2022], Burroni et al. [2023].

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But we got good results with D_θ as high as $15,098$ using only only $N = 30$. Why?

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Some first steps

Theorem [Giordano et al., 2023]: When $\mathcal{P}(\theta|y)$ is multivariate normal, and we use the mean-field Gaussian approximation, then, for any particular entry η_d of η, then $\left|\hat{\eta}_d - \overset{*}{\eta}_d\right| = O_p(N^{-1/2})$ irrespective of D_θ.

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Theorem [Giordano et al., 2023]: Assume $\mathcal{P}(\theta|y)$ has a "global-local" structure:

$$\theta = (\gamma, \lambda_1, \ldots, \lambda_{D_\lambda}) \qquad \mathcal{P}(\gamma, \lambda_1, \ldots, \lambda_{D_\lambda}|y) = \prod_{d=1}^{D_\lambda} \mathcal{P}(\gamma, \lambda_d|y).$$

Assume that the dimension of γ and each λ_d stays fixed as D_λ grows.

Under regularity conditions, the DADVI error scales as $\sqrt{\log D_\lambda / N}$, not $\sqrt{D_\lambda / N}$.

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Assume that the dimension of γ and each λ_d stays fixed as D_λ grows.

Under regularity conditions, the DADVI error scales as $\sqrt{\log D_\lambda / N}$, not $\sqrt{D_\lambda / N}$.

Proposal: The "in general" analysis of [Nemirovski et al., 2009] is too general for many practically interesting BBVI problems.

A negative result for expressive approximations

Theorem [Giordano et al., 2023]: Assume that $N < D_\theta$, and that we use a full-rank Gaussian approximation. Then the DADVI objective is unbounded below, and optimization of the DADVI objective will approach a degenerate point mass at $\mathrm{argmax}_\theta \log \mathcal{P}(\theta|y)$.

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Proof sketch: For any value of the variational mean, the DADVI objective only depends on $\mathcal{P}(\theta|y)$ evaluated in a subspace spanned by $\mathcal{Z}_N$. The variational objective can be driven to $-\infty$ by driving the variance to zero in the subspace orthogonal to $\mathcal{Z}_N$.

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Proposal: All sufficiently expressive variational approximations (e.g. normalizing flows) will fail in the same way in high dimensions. However, this pathology can be obscured and overlooked in practice by low-quality optimization.

Conclusion

Black Box Variational Inference with a Deterministic Objective: Faster, More Accurate, and Even More Black Box.

Giordano, R.*, Ingram, M.*, Broderick, T. (* joint first authors), 2023.

(Arxiv preprint here.)

- By fixing the randomness in the ADVI objective, DADVI provides BBVI that is easier to use, faster, and more accurate than stochastic gradient.
- The approximation used by DADVI will not work in high dimensions for sufficiently expressive approximating distributions (e.g., full-rank ADVI).
- There appears to be a gap between the optimization literature and BBVI practice in high dimensions for a class of practically interesting problems.

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Supplemental material

Linear response covariances

Posterior variances are often badly estimated by mean-field (MF) approximations.

Example: With a correlated Gaussian $\mathcal{P}(\theta|y)$ with ADVI, the ADVI means are correct, but the ADVI variances are underestimated.

Take a variational approximation $\overset{*}{\eta} := \mathrm{argmin}_{\eta \in \mathbb{R}^{D_\eta}} \mathrm{KL}_{\mathrm{VI}}(\eta)$. Often,

$$\underset{\mathcal{Q}(\theta|\overset{*}{\eta})}{\mathbb{E}}[\theta] \approx \underset{\mathcal{P}(\theta|y)}{\mathbb{E}}[\theta] \quad \text{but} \quad \underset{\mathcal{Q}(\theta|\overset{*}{\eta})}{\mathrm{Var}}(\theta) \neq \underset{\mathcal{P}(\theta|y)}{\mathrm{Var}}(\theta). \tag{1}$$

Example: Correlated Gaussian $\mathcal{P}(\theta|y)$ with ADVI.

Linear response covariances use the fact that, if $\mathcal{P}(\theta|y,t) \propto \mathcal{P}(\theta|y)\exp(t\theta)$, then

$$\left.\frac{d \underset{\mathcal{P}(\theta|y,t)}{\mathbb{E}}[\theta]}{dt}\right|_{t=0} = \underset{\mathcal{P}(\theta|y)}{\mathrm{Cov}}(\theta). \tag{2}$$

Let $\overset{*}{\eta}(t)$ be the variational approximation to $\mathcal{P}(\theta|y,t)$, and take

$$\underset{\mathcal{Q}(\theta|\overset{*}{\eta})}{\mathrm{LRCov}}(\theta) = \left.\frac{d \underset{\mathcal{Q}(\theta|\overset{*}{\eta}(t))}{\mathbb{E}}[\theta]}{dt}\right|_{t=0} = \left(\nabla_\eta \underset{\mathcal{Q}(\theta|\overset{*}{\eta})}{\mathbb{E}}[\theta]\right) \left(\nabla^2_\eta \mathrm{KL}_{\mathrm{VI}}\left(\overset{*}{\eta}\right)\right)^{-1} \left(\nabla_\eta \underset{\mathcal{Q}(\theta|\overset{*}{\eta})}{\mathbb{E}}[\theta]\right)$$

Example: For ADVI with a correlated Gaussian $\mathcal{P}(\theta|y)$, $\underset{\mathcal{Q}(\theta|\overset{*}{\eta})}{\mathrm{LRCov}}(\theta) = \underset{\mathcal{Q}(\theta|\overset{*}{\eta})}{\mathrm{Cov}}(\theta)$.